Graph neural networks: Advanced topics

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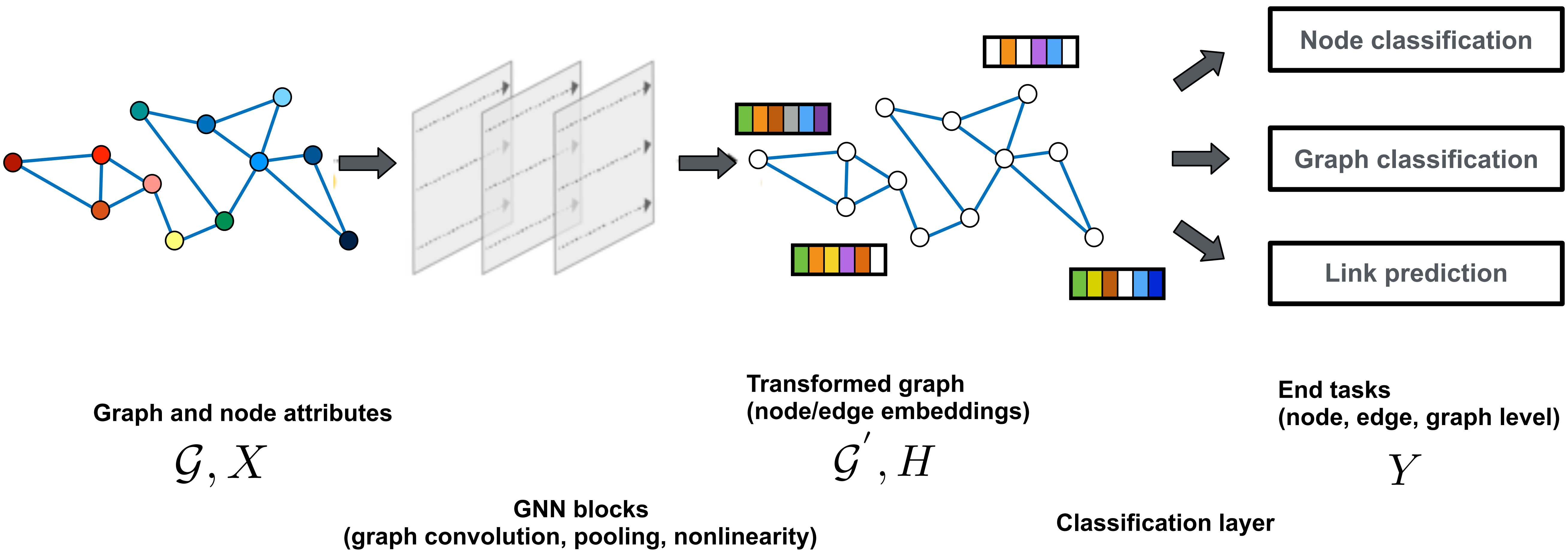
May 15, 2023

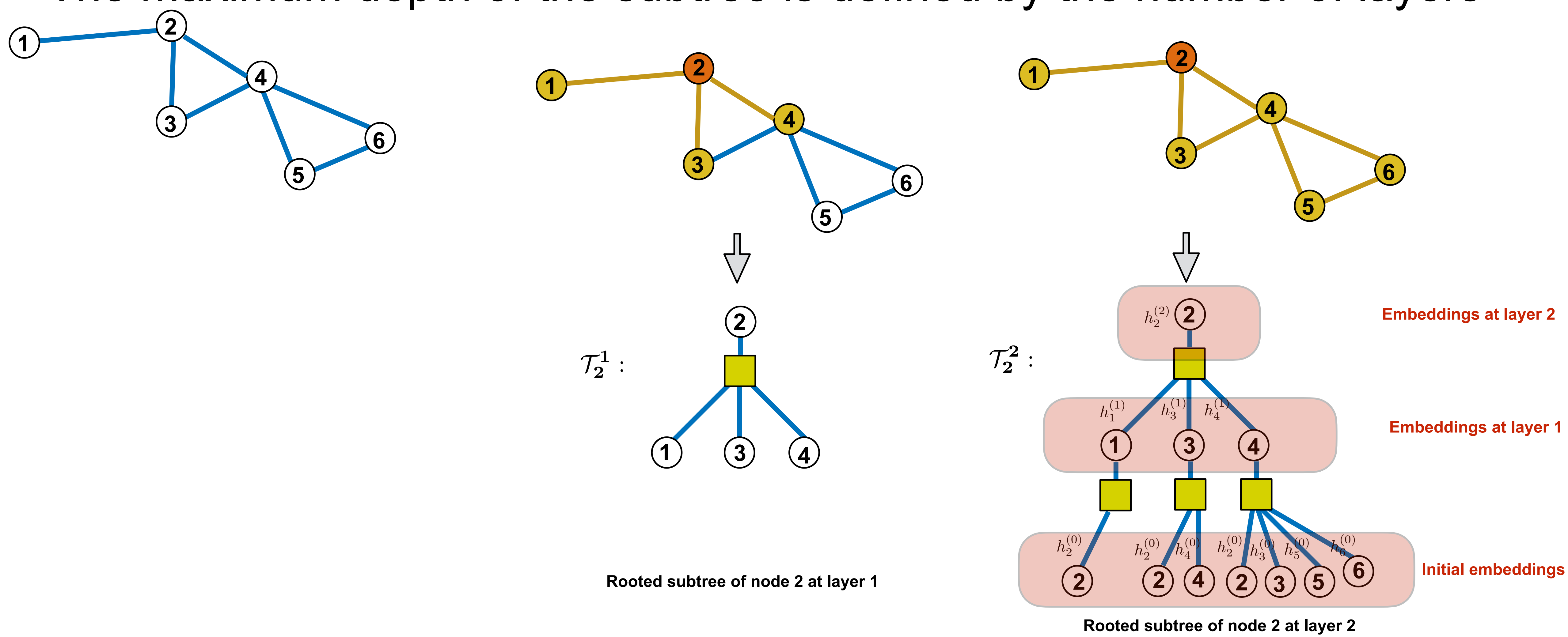
Recap: Graph neural networks (GNNs)

- A different way of obtaining ‘deeper’ embeddings inspired by deep learning
- They generalize to graphs with node attributes



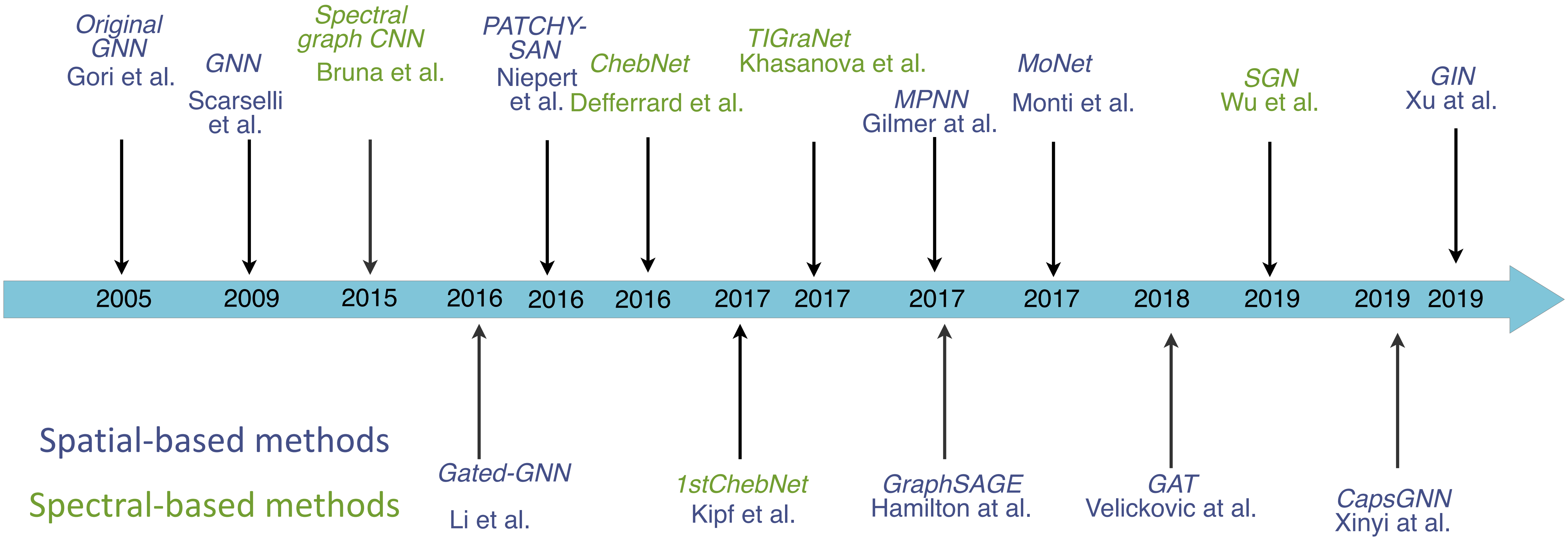
From graphs to rooted subtrees

- Each subgraph can be mapped to a rooted subtree or a subtree pattern
- The maximum depth of the subtree is defined by the number of layers



Different rooted subtrees should be assigned different node embeddings!

Recap: First GNN architectures



- Recent trends
  - Spectrally-inspired architectures: GraphHeat (Xu'19), GWNN (Xu'19), SIGN (Frasca'20), DGN (Beaini'20), Framelets (Zheng'21), FAGCN (Bo'21)
  - More expressive GNNs: higher order WL test (Maron'19, Morris'20), physics-inspired GNNs (Chamberlain'21), and many more!

Outline

- Expressive power of GNNs
- Inferring the graph topology
- Dynamic graph models
- Learning with sparse labels

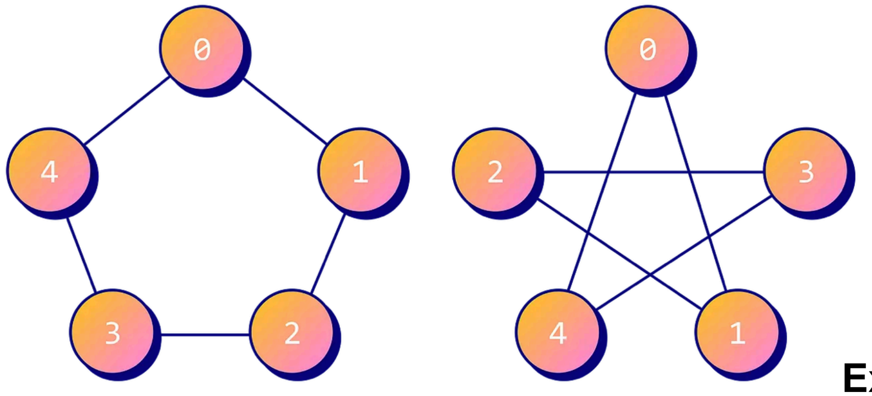
Outline

- **Expressive power of GNNs**
- Inferring the graph topology
- Dynamic graph models
- Learning with sparse labels

Representation power of MPNNs

- Typically done by analysing how expressive a GNN is in learning to represent and **distinguish between different graph structures**

- This implies solving the graph isomorphism problem:
  - Two graphs are isomorphic if there exists an index permutation between the nodes that preserve node adjacencies (NP hard)
  - Isomorphic graphs should be mapped to the same representation and non-isomorphic ones to different representations

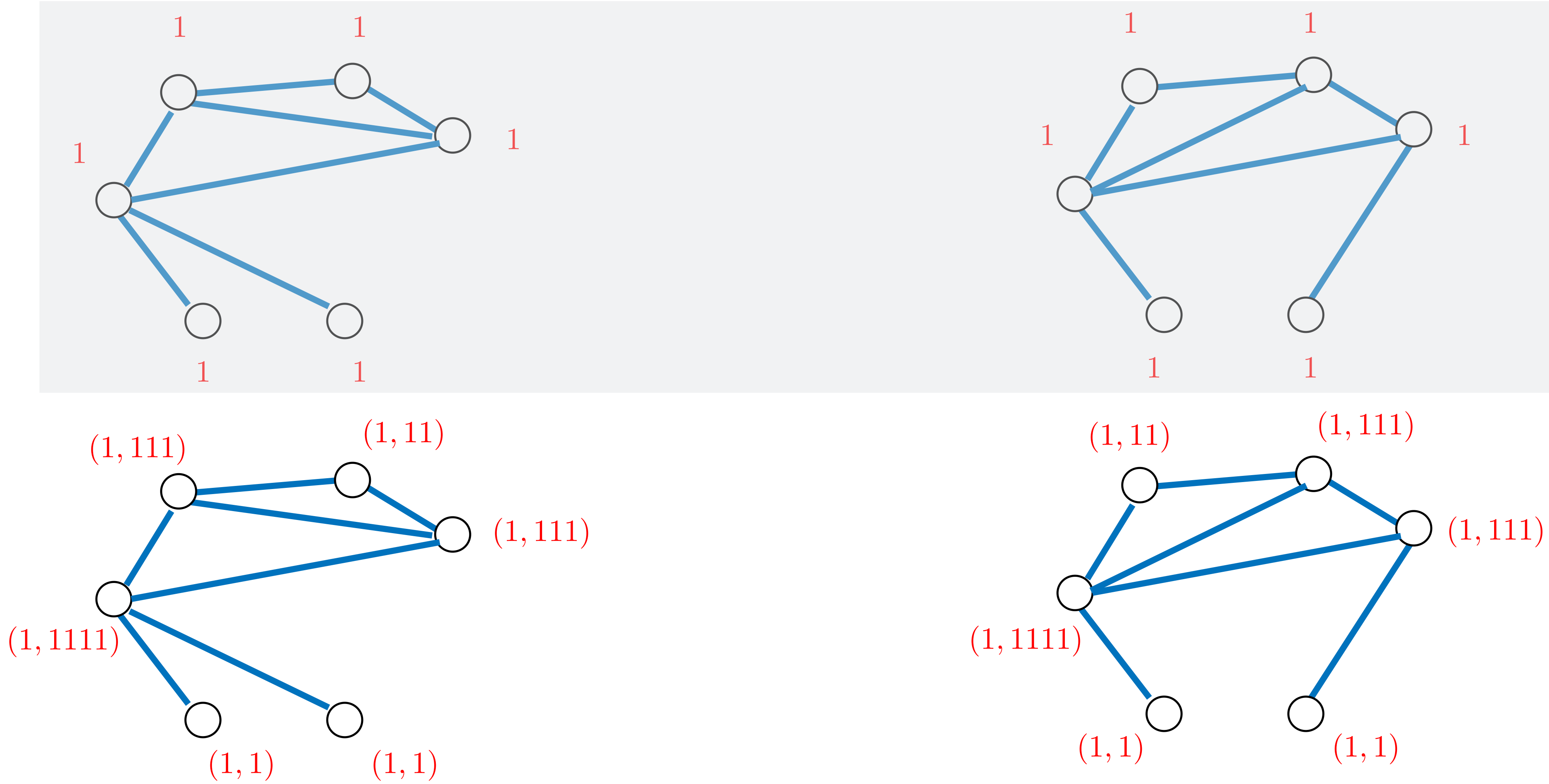


Example of two isomorphic graphs

Recall the WL kernel

Initial colors

Recall the WL kernel



Initial colors

Aggregate neighbourhood colors

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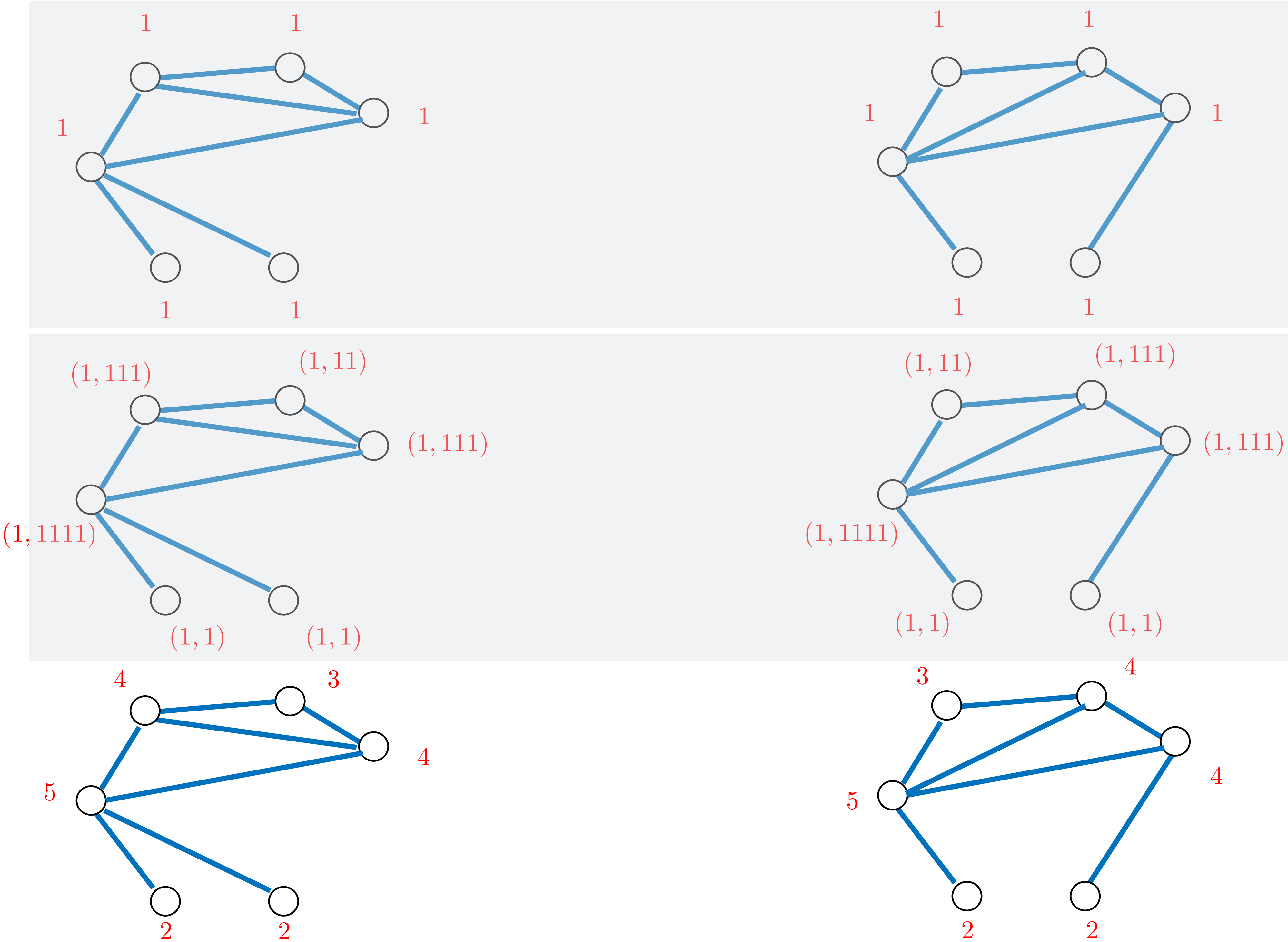


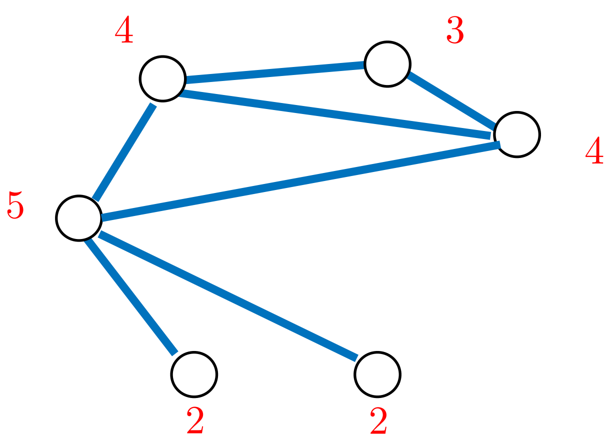
Initial colors

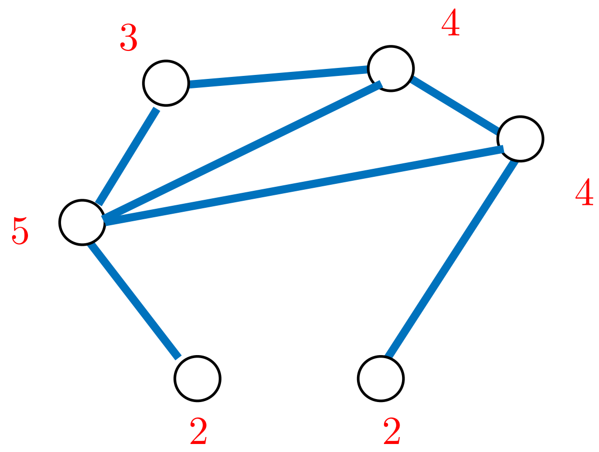
Aggregate neighbourhood colors

Hash table

$(1, 1)$	$\rightarrow$	2
$(1, 11)$	$\rightarrow$	3
$(1, 111)$	$\rightarrow$	4
$(1, 1111)$	$\rightarrow$	5

Recall the WL kernel





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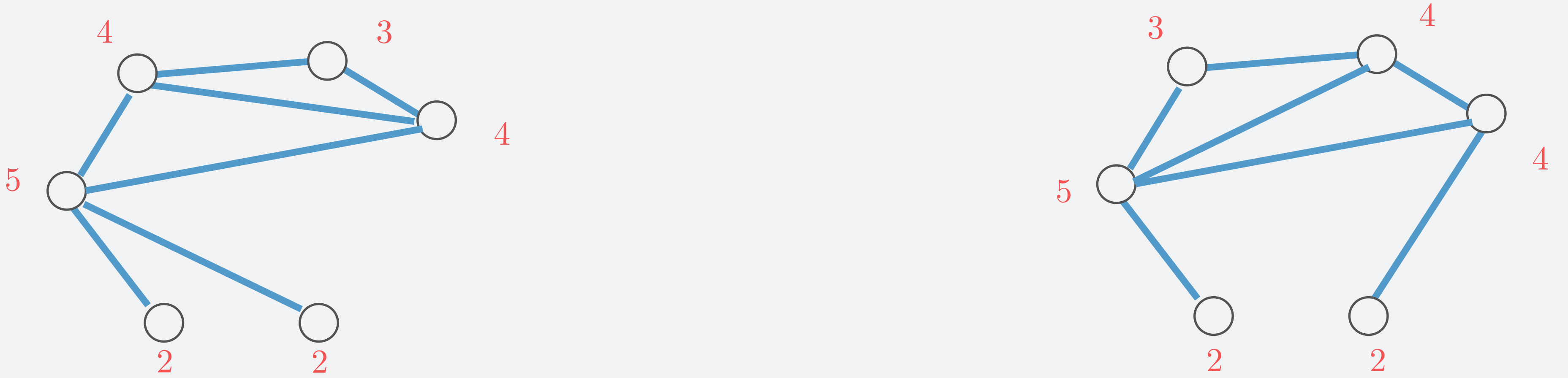

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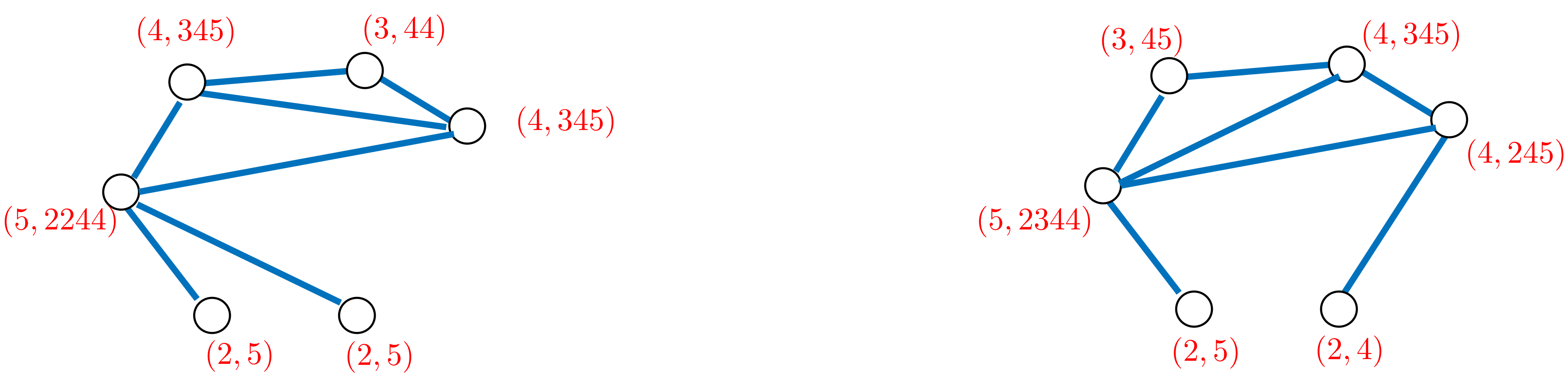

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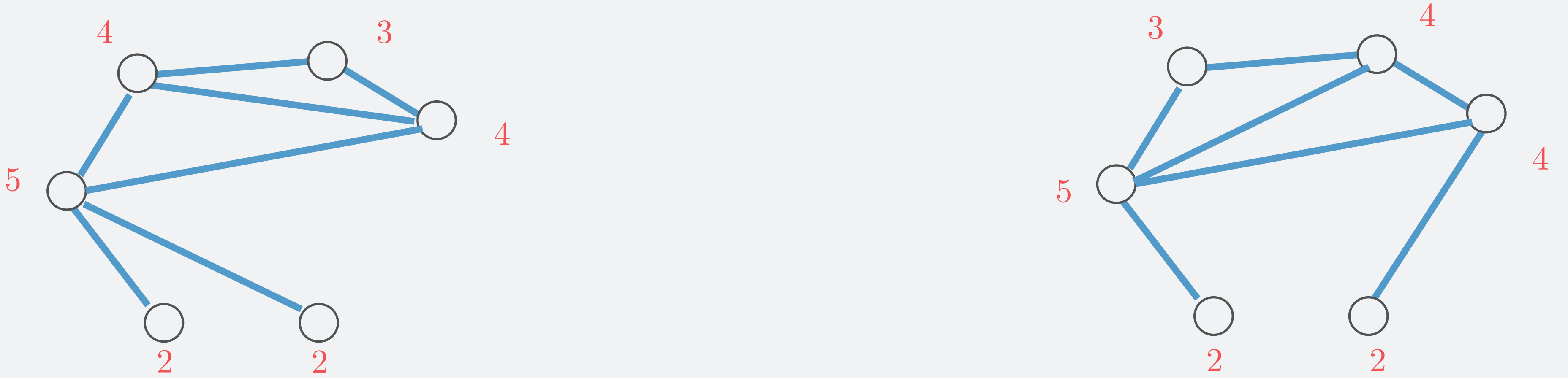

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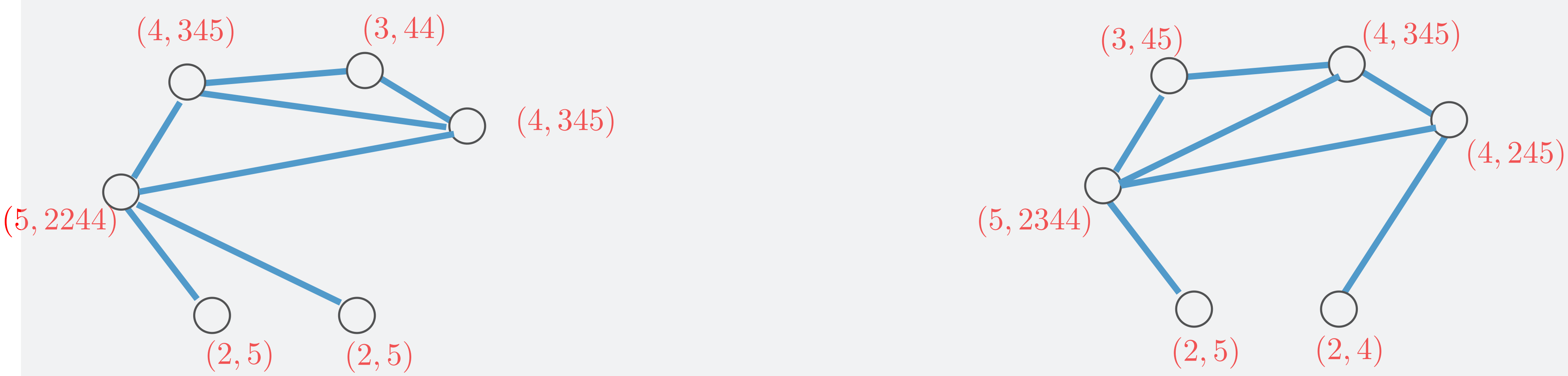

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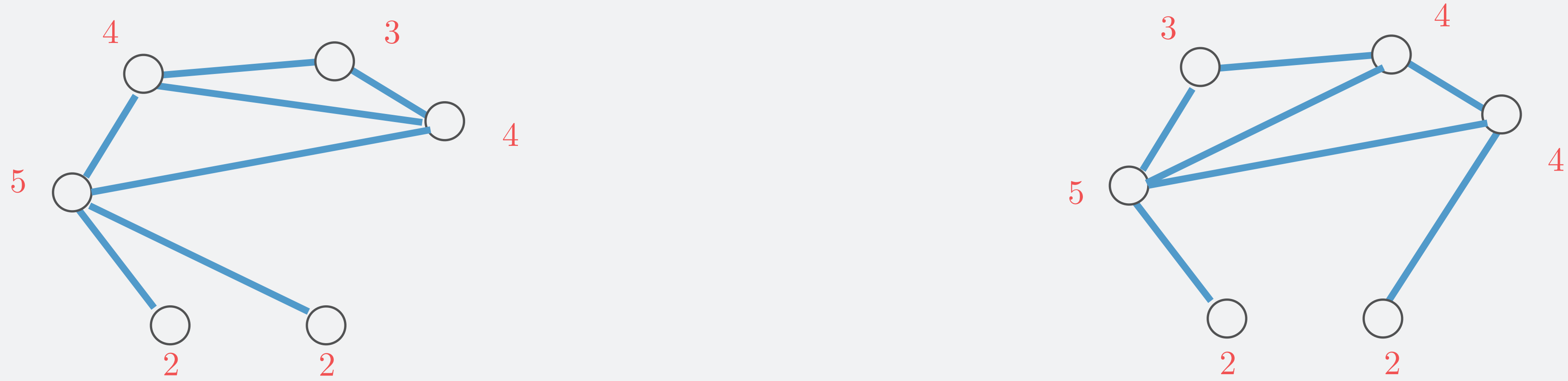

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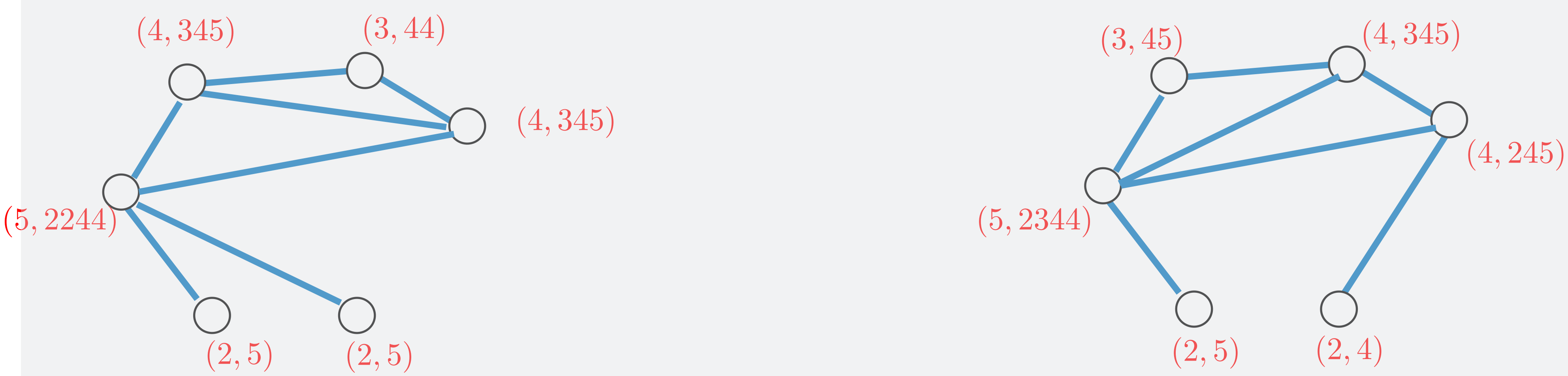
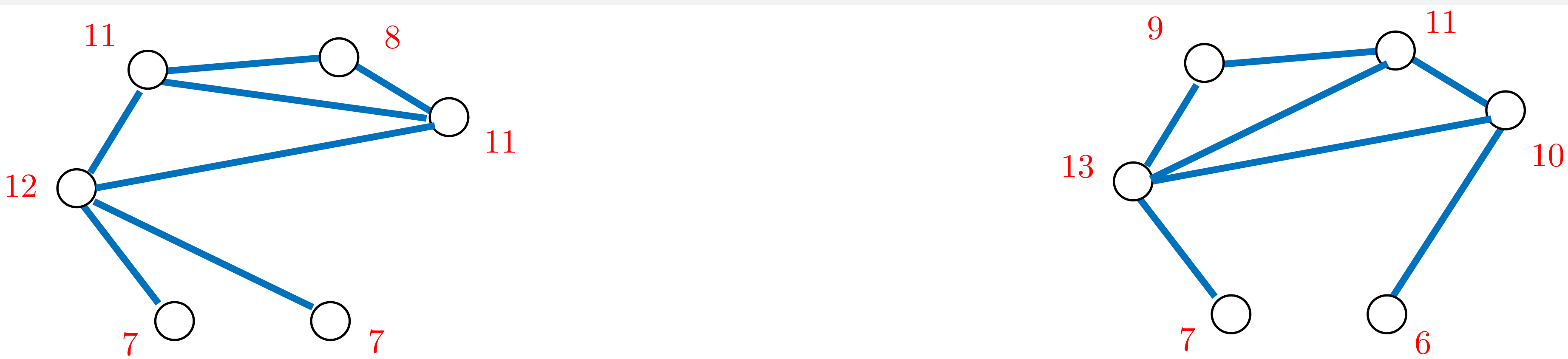


Aggregate neighbourhood colors

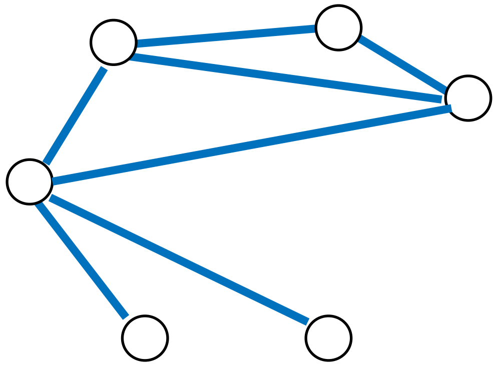


Hash table

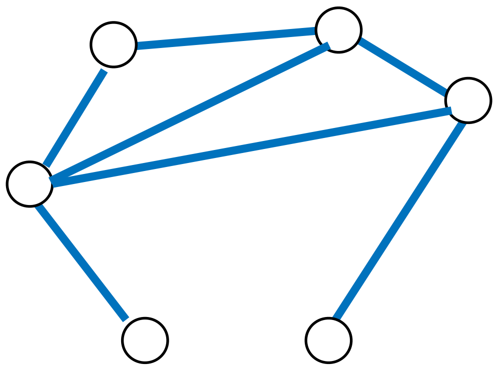
$(2, 4)$	$\rightarrow$	6
$(2, 5)$	$\rightarrow$	7
$(3, 44)$	$\rightarrow$	8
$(3, 45)$	$\rightarrow$	9
$(4, 245)$	$\rightarrow$	10
$(4, 345)$	$\rightarrow$	11
$(5, 2244)$	$\rightarrow$	12
$(5, 2344)$	$\rightarrow$	13

Recall the WL kernel

- After K iterations, the WL kernel computes the histogram of colors



$$\begin{matrix} & 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13 \\ \phi(\mathcal{G}_1) = & [6, 2, 1, 2, 1, 0, 2, 1, 0, 0, 2, 1, 0] \end{matrix}$$



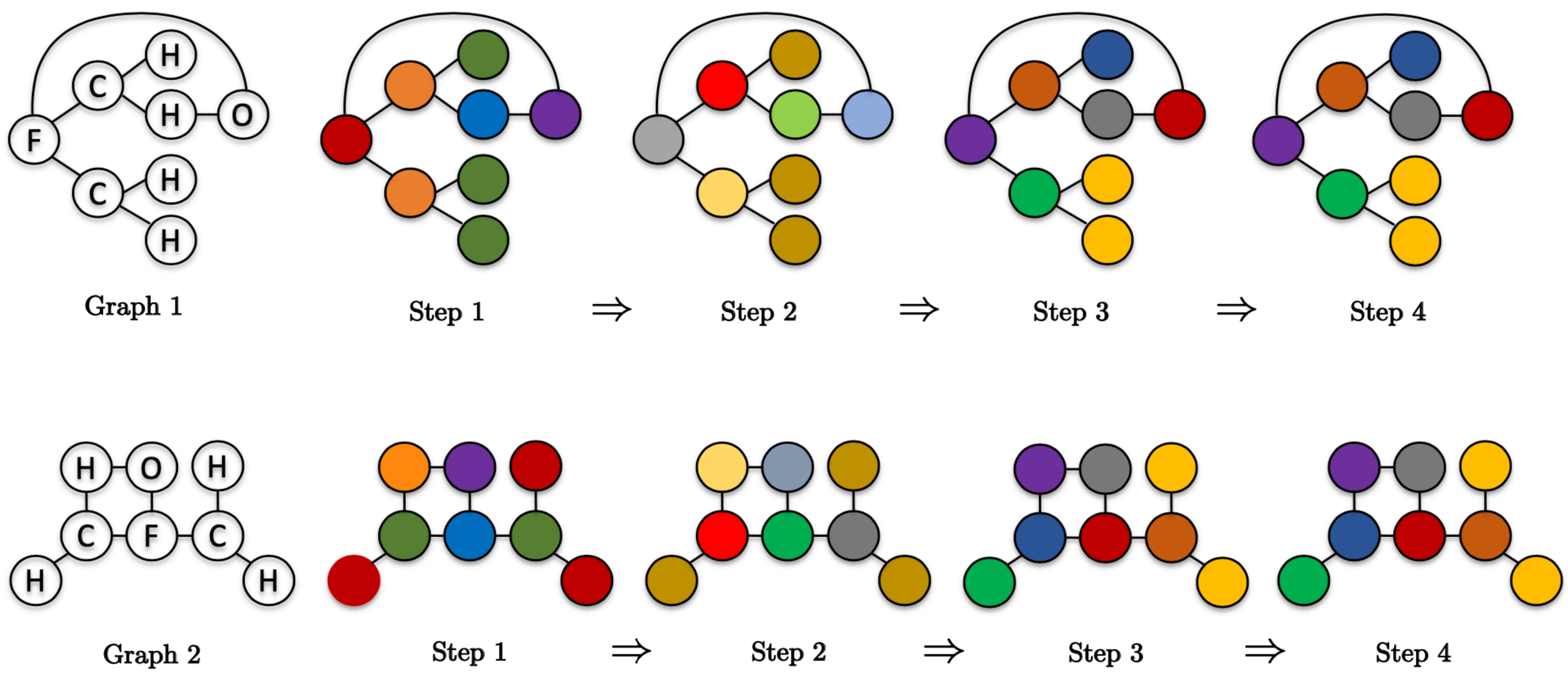
$$\begin{matrix} & 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13 \\ \phi(\mathcal{G}_2) = & [6, 2, 1, 2, 1, 1, 1, 0, 1, 1, 1, 0, 1] \end{matrix}$$

WL kernel

$$K(\mathcal{G}_1, \mathcal{G}_2) = < \phi(\mathcal{G}_1), \phi(\mathcal{G}_2) >$$

Strong connections with 1-WL test (1)

- 1-Weisfeiler-Lehman (WL) is a classical algorithm for graph isomorphism
- It tells you if two graphs are not isomorphic, but it does not allow you to conclude if they are isomorphic (necessary but not sufficient condition)



- By construction, GNNs can only be as powerful as the 1-WL test

[Illustrative example from X. Bresson]

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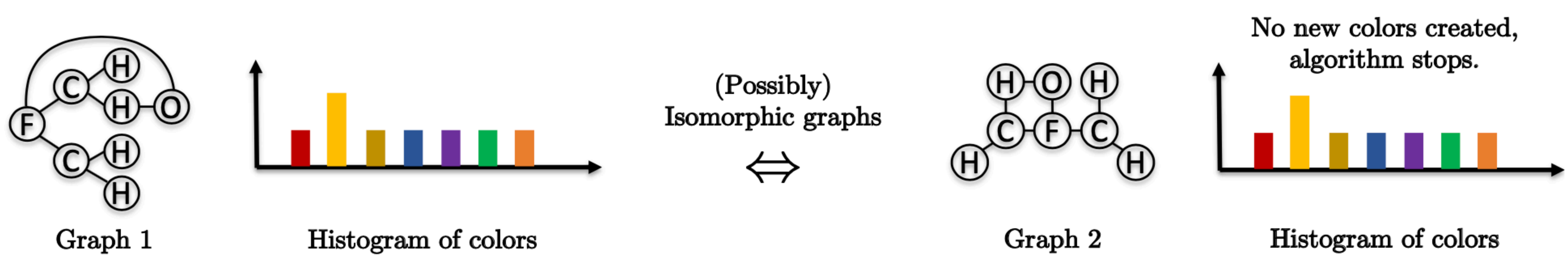

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[Illustrative example from X. Bresson]

Strong connections with 1-WL test (2)

- MPNNs are equivalent to (at most as powerful as) the 1-WL isomorphism test
  - WL function should be injective: different inputs are mapped to different outputs
  - GINs are as powerful as the 1-WL test

1-WL test

- **Input:** a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, W)$
- Assign an initial color c_i^0 (e.g., node degree) to each node i of $\mathcal{V}$
- For each iteration $l+1$ refine node colors as

$$c_i^{l+1} = \mathrm{HASH}\big(\{c_i^l, \{c_j^l\}_{j \in \mathcal{N}_i}\}\big)$$

- Until stable node coloring is reached
- **Output:** The node colors $\{c_i^{l_{max}}\}_{i=\{1,2,\ldots,N\}}$

MPNN

- **Input:** a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, W)$
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- Over discrete features, GNNs can only be as powerful as the 1-WL test

[Xu et al., How powerful are graph neural networks, ICLR 2019]

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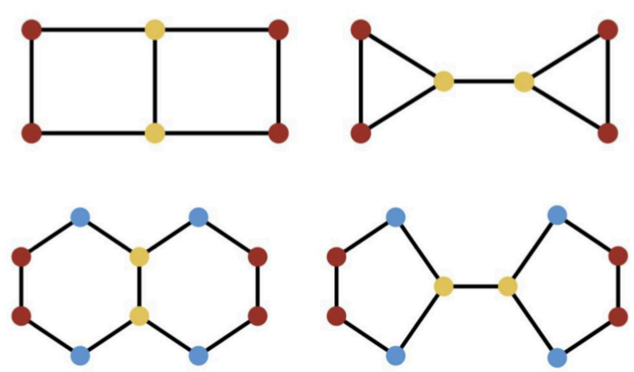
Limitations of MPNNs

- A lot of works have shown that MPNNs have some limitations, e.g., [Morris'19, Xu'18, Chen'20]
  - They fail to capture long run interactions

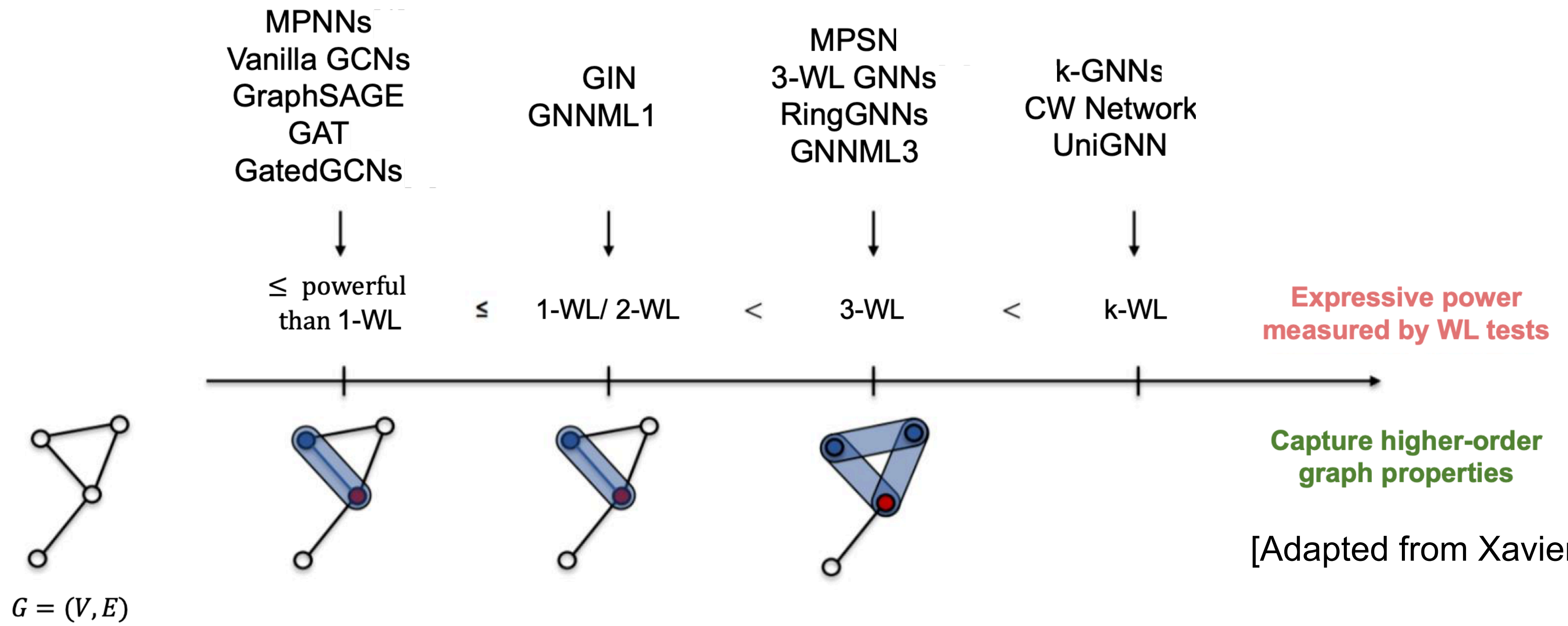
  - They fail to distinguish higher-order structures (similar to WL)



- There are non-isomorphic subgraphs that are considered equivalent by MPNNs

Improvements of expressiveness of MPNNs

- **Intuition:** Design algorithms inspired from higher-dimensional isomorphism tests (k-WL induced GNNs)



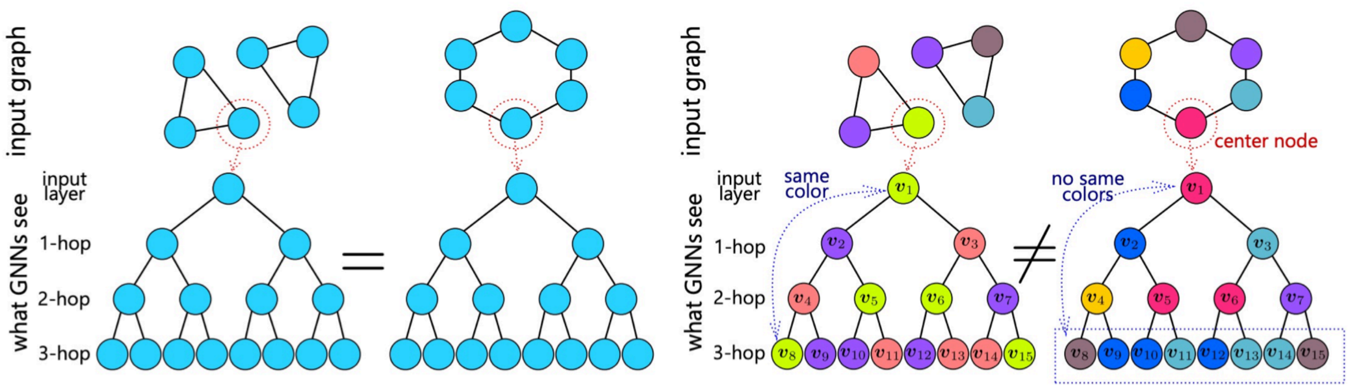
[Adapted from Xavier Bresson's slides]

✓ These models are more expressive

- They (often) loose the advantage of locality and linear complexity of MPNNs

Improvements of expressiveness of MPNNs

- **Intuition:** Exploit the identity of each node or a neighborhood around it to increase the expressive power of MPNNs
  - Augment nodes with randomized/positional features or local context (positional encoding)
  - Examples: [Loukas'20, Vignac'20, Sato'21, Abboud'21]



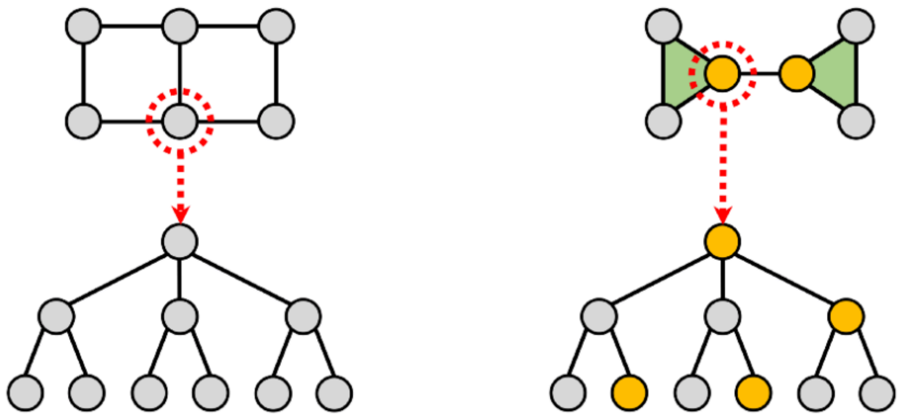
(a) Identical Features. (b) Random Features.

✓ These models are more expressive

- They are either not permutation equivariant or computationally costly

Improvements of expressiveness of MPNNs

- **Intuition:** If the network cannot detect a pattern, we can count this pattern and add the extra count as an additional feature
  - Augment nodes with handcrafted subgraph-based features (structural encoding)
  - Examples: [Bouritsas'20]



✓ These models are at least as expressive as 1-WL and they can distinguish some non-isomorphic graphs that 1-WL fails

- They require expert knowledge on what features are relevant for a task

Still MPNNs remain the most widely-used framework in practice!

Outline

- Expressive power of GNNs
- **Inferring the graph topology**
- Dynamic graph models
- Learning with sparse labels

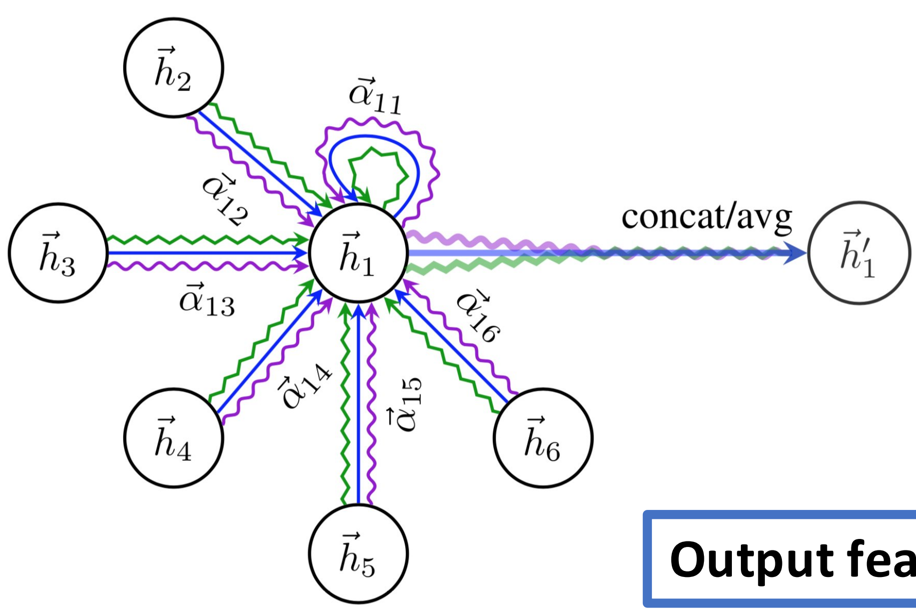
What if the graph is not given

- All techniques so far require a graph to be provided as input
- In many applications, the graph is not given
- A fully connected graph could be designed, but:
  - It does not capture important interactions between nodes
  - It does not scale

How can we learn a graph from data in a GNN?

Graph attention can be considered as an example of graph inference

- For a given connectivity matrix, attentional GNNs learn the weights of each edge
  - Different weights are attributed to different nodes in a neighbourhood
  - Dependence on the global graph structure can be removed



Output features

Updated embedding

$$h_i^{l+1} = \sigma(\alpha_{ii}^l \theta_0^l h_i^l + \sum_{j \in \mathcal{N}_i} \alpha_{ij}^l \theta_1^l h_j^l)$$

[Velickovic et al., Graph Attention Networks, ICLR 2018]

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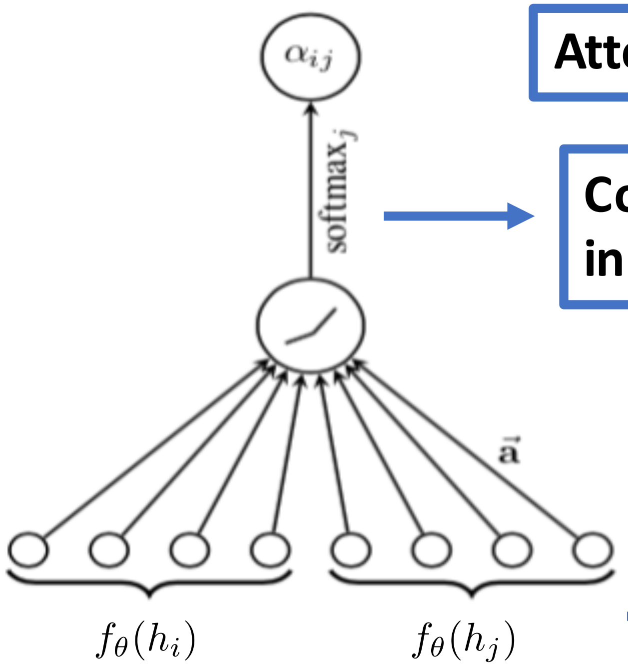


Attention weights

Comparison of input features

Input features of nodes i, j

Updated embedding

$$h_i^{l+1} = \sigma(\alpha_{ii}^l \theta_0^l h_i^l + \sum_{j \in \mathcal{N}_i} \alpha_{ij}^l \theta_1^l h_j^l)$$

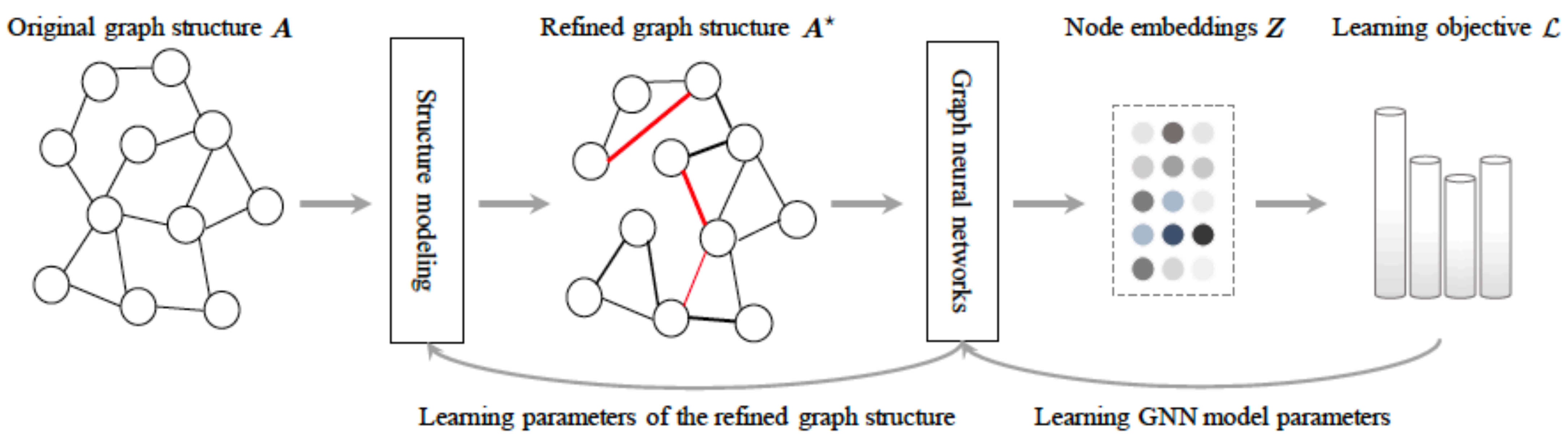
$$\alpha_{ij}^{l+1} = \alpha\left(f_\theta(h_i^{l+1}), f_\theta(h_j^{l+1})\right)$$

Updated edge attention

[Velickovic et al., Graph Attention Networks, ICLR 2018]

Learning the connectivity

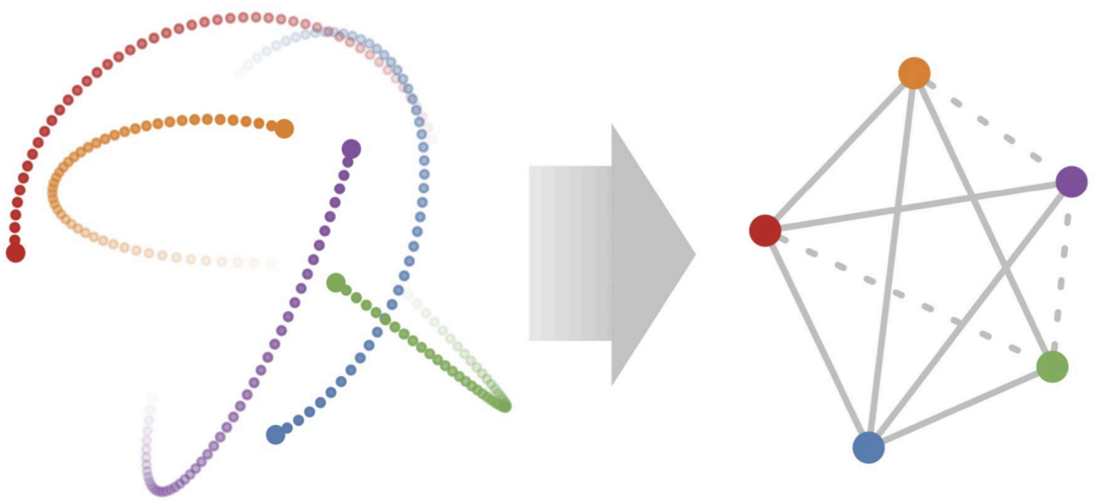
- We can infer simultaneously the graph structure and the node representations by optimising a downstream task



[Zhu et al., Deep Graph Structure Learning for Robust Representations: A Survey, arXiv, 2021]

Example: Neural relational inference

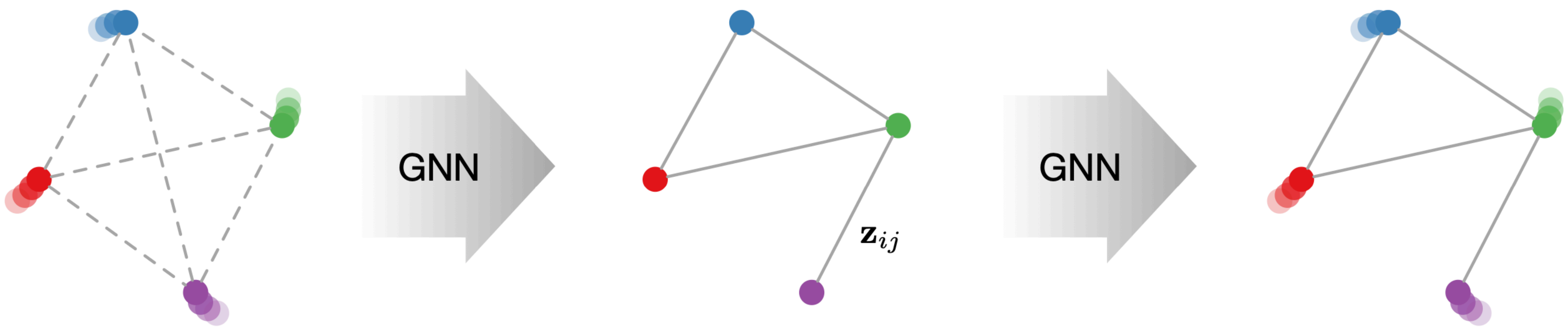
- Objective: Infer the interaction graph from observed dynamics without knowing structure of interactions



- Intuition: Use a downstream task to drive graph construction
  - Infer the graph through an encoder
  - Use the graph to make predictions
  - Optimize the entire system end-to-end

[Kipf et al., Neural relational inference for interacting systems, ICML 2018]

Example: Neural relational inference



Observe dynamics

$\mathbf{x} = (\mathbf{x}^1, \ldots, \mathbf{x}^T)$

Interaction graph proposal

$\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})$

Reconstruct dynamics*

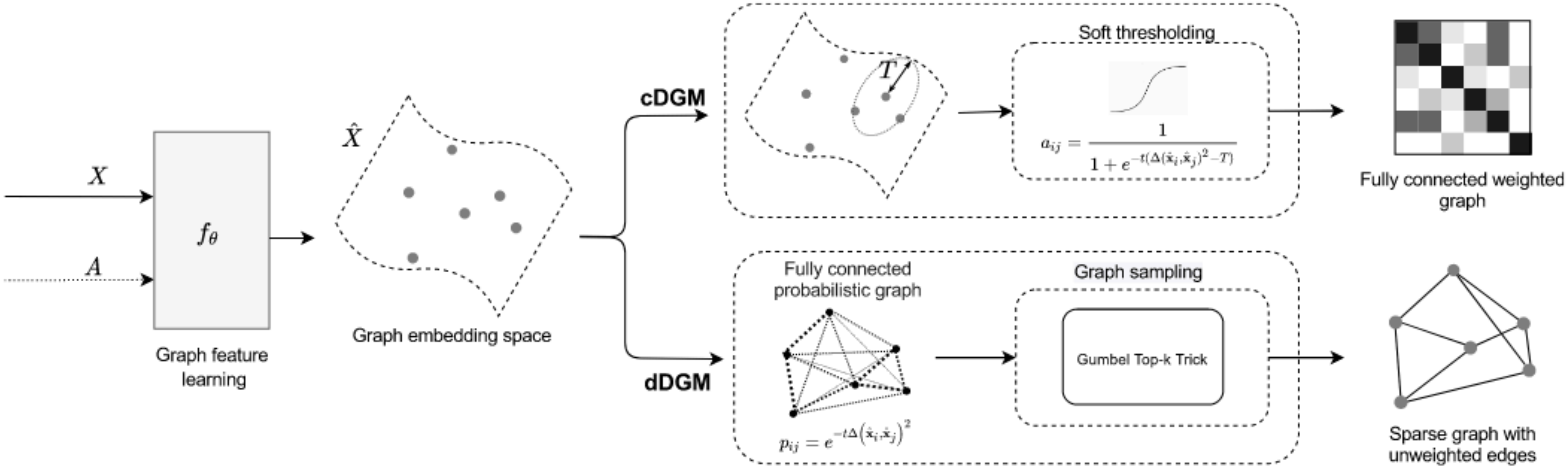
$p_\theta(\mathbf{x}|\mathbf{z})$

VAE Objective (ELBO) $\mathcal{L} = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathrm{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})]$

Reconstruction **Regularization**

Example: Differential graph module

- DGM projects nodes to a latent space and uses a Gaussian kernel to obtain a probability for each node pair
- The learnable function predicting the probability is optimized for a downstream task



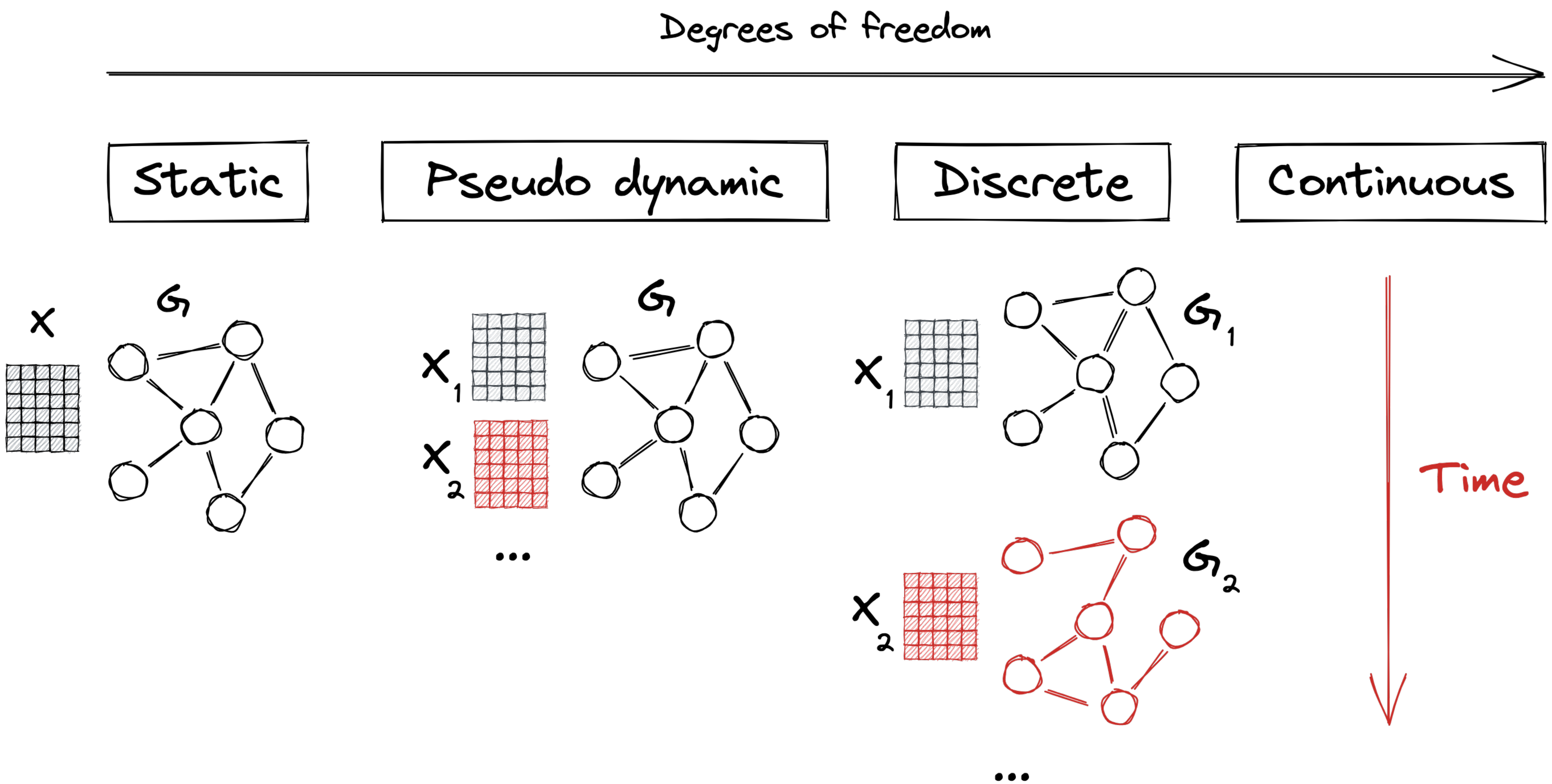
[Kazi et al., Differentiable graph module for graph convolutional networks, ICML, 2020]

Outline

- Expressive power of GNNs
- Inferring the graph topology
- **Dynamic graph models**
- Learning with sparse labels

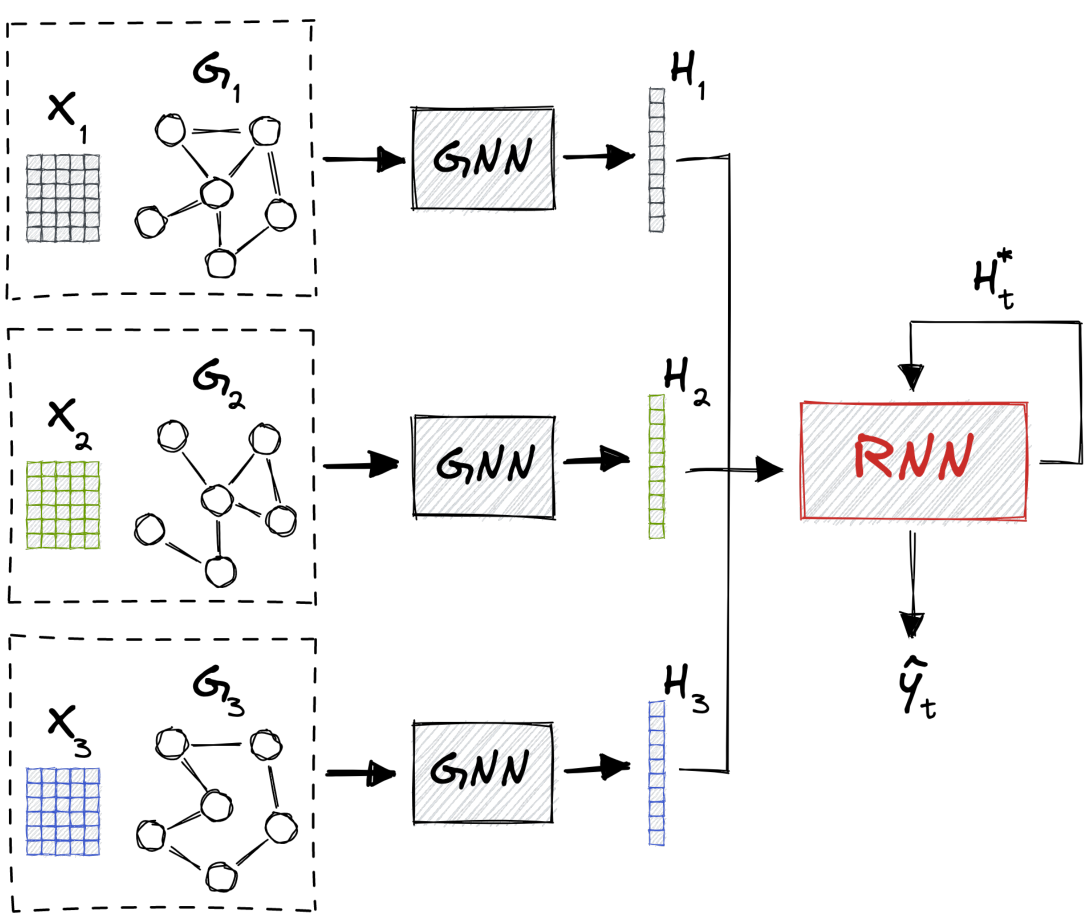
Spatial-temporal GNNs

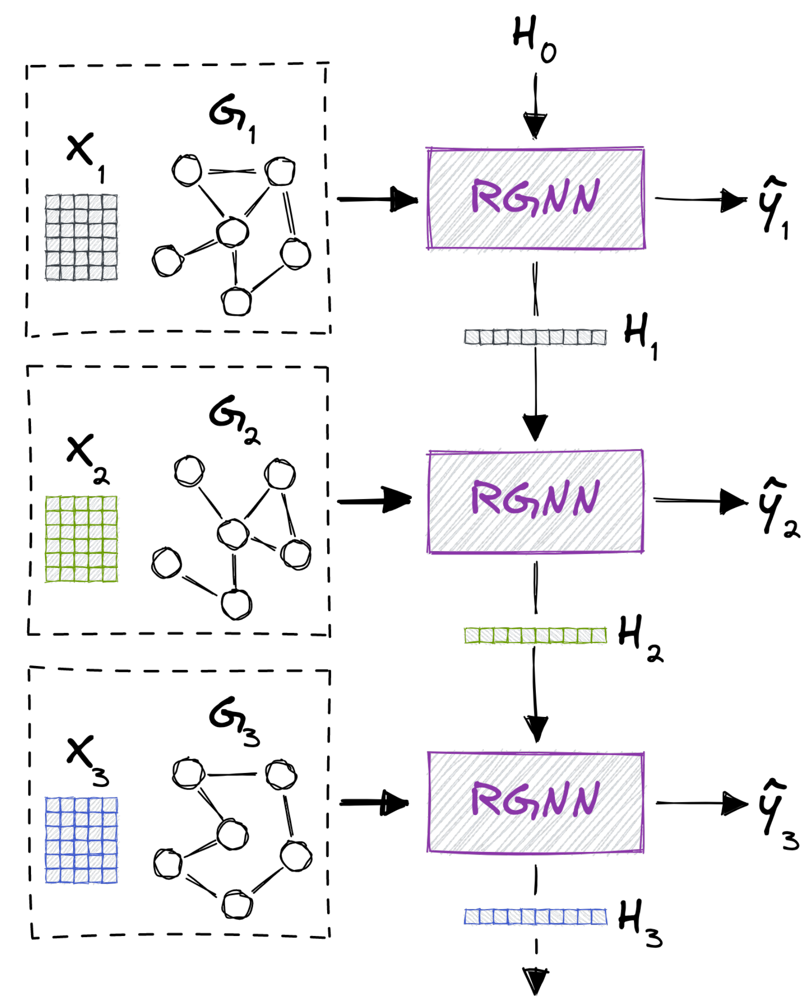
- Dynamic networks are graphs where over time links and nodes may appear and disappear, and features may change



[Slide from W. Cappelletti]

Temporal GNNs follow two paradigms





Spatial then temporal:

Node embeddings for each time step are fed to a temporal model

Spatio-temporal:

A single model for embedding spatial and temporal information

[Skarding et al., Foundations and Modeling of Dynamic Networks Using Dynamic Graph Neural Networks: A Survey, IEEE Access, 2021]

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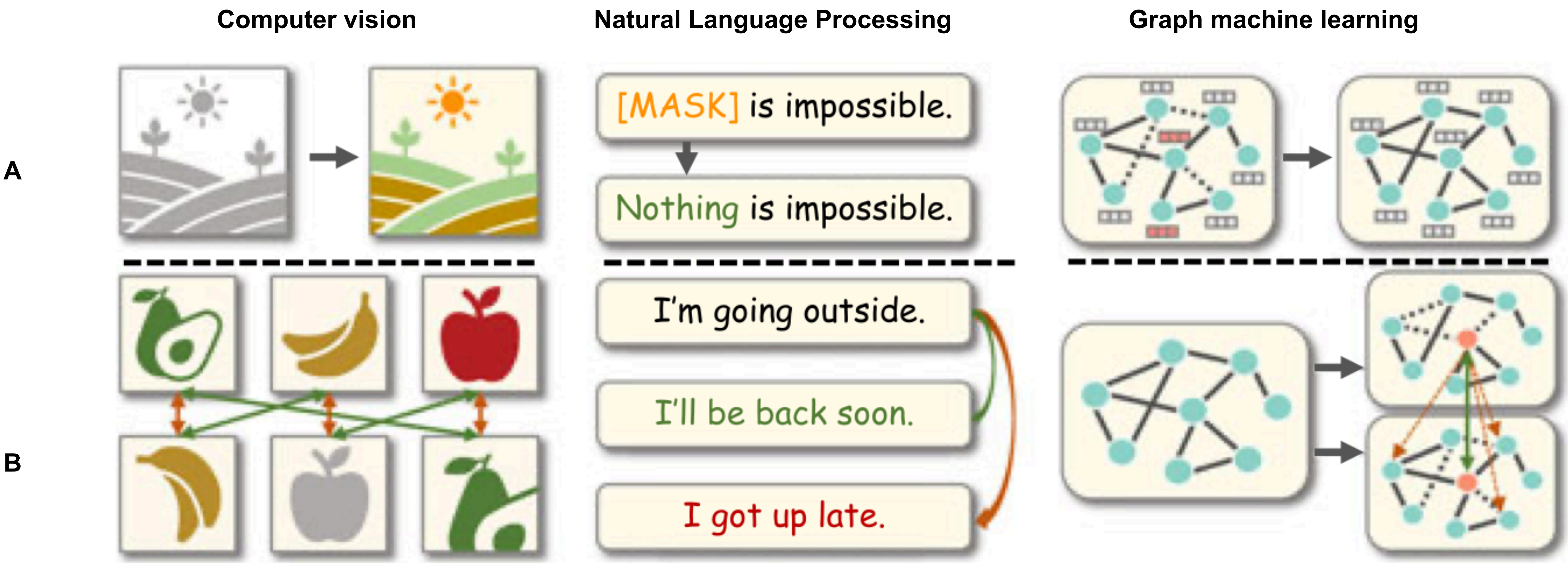
Unsupervised/self-supervised learning with GNNs

- So far, we have assumed that labels are available
  - They are used to design a loss function
- What if the labels are not available or limited?
  - Loss function should depend on the information provided by the graph itself: e.g., input features, graph topology
  - Some examples: DeepWalk, node2vec, SDNE (they consider only the graph structure)
- In self-supervised learning (SSL), models are learned by solving a series of hand-crafted auxiliary tasks (so-called pretext tasks)
  - Supervision signals are acquired from data itself, without the need for annotation

Illustrative examples of pretext tasks



A. Image colorisation
B. Image contrastive learning

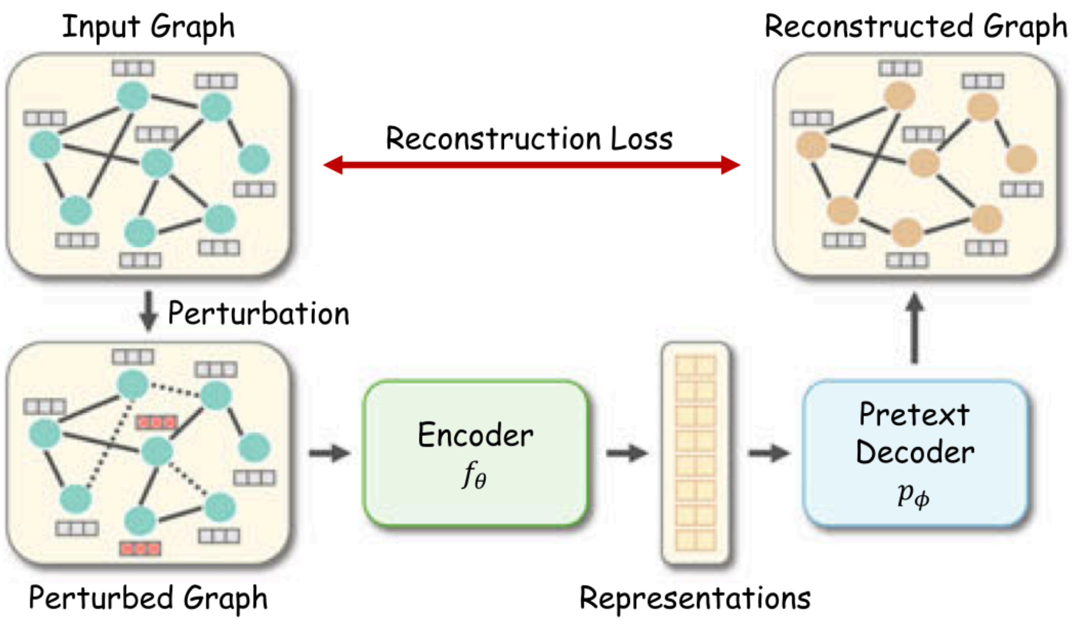
A. Masked language modelling
B. Next sentence prediction

A. Masked graph generation
B. Node contrastive learning

[Liu et al., Graph Self-Supervised learning: A survey, IEEE TKDE 2023]

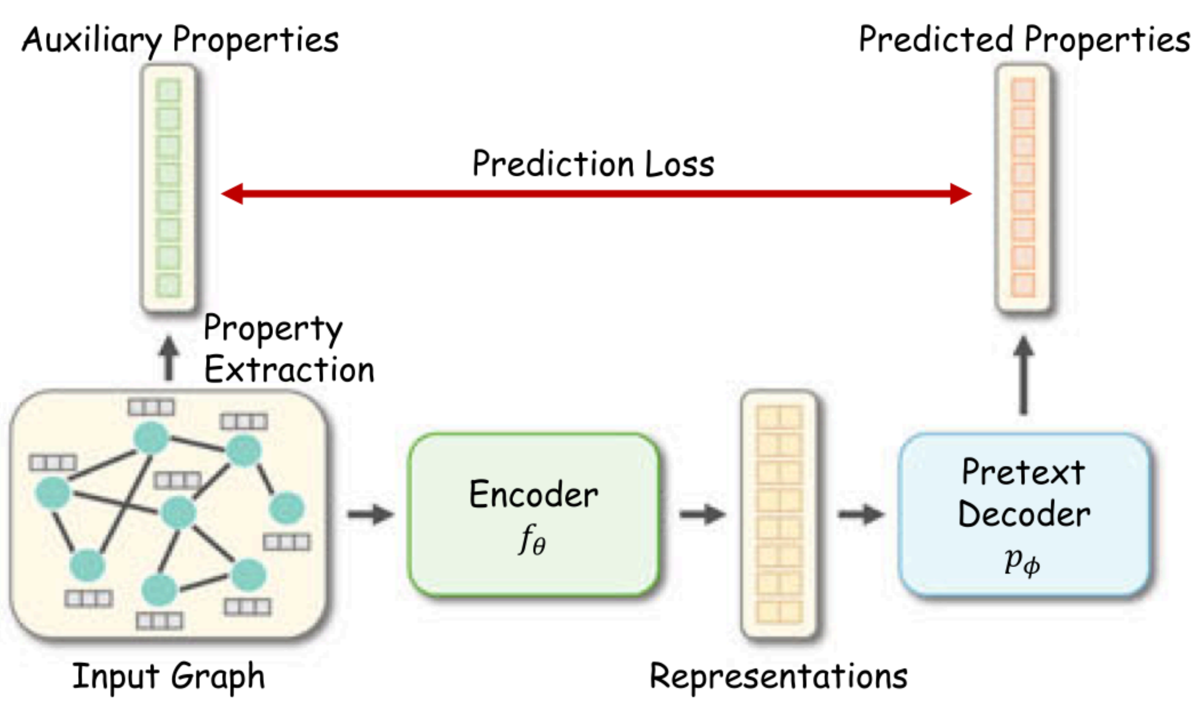
Generation-based SSL

- Pretext tasks are defined as a graph data reconstruction problem of either the graph structure or the node attributes
- GNNs are typically used to encode nodes in the graph (encoder)
- The decoder reconstructs the adjacency matrix or the node attributes (pretext task)
- The loss is defined to measure the difference between the reconstructed and the original graph data (e.g., GAE)



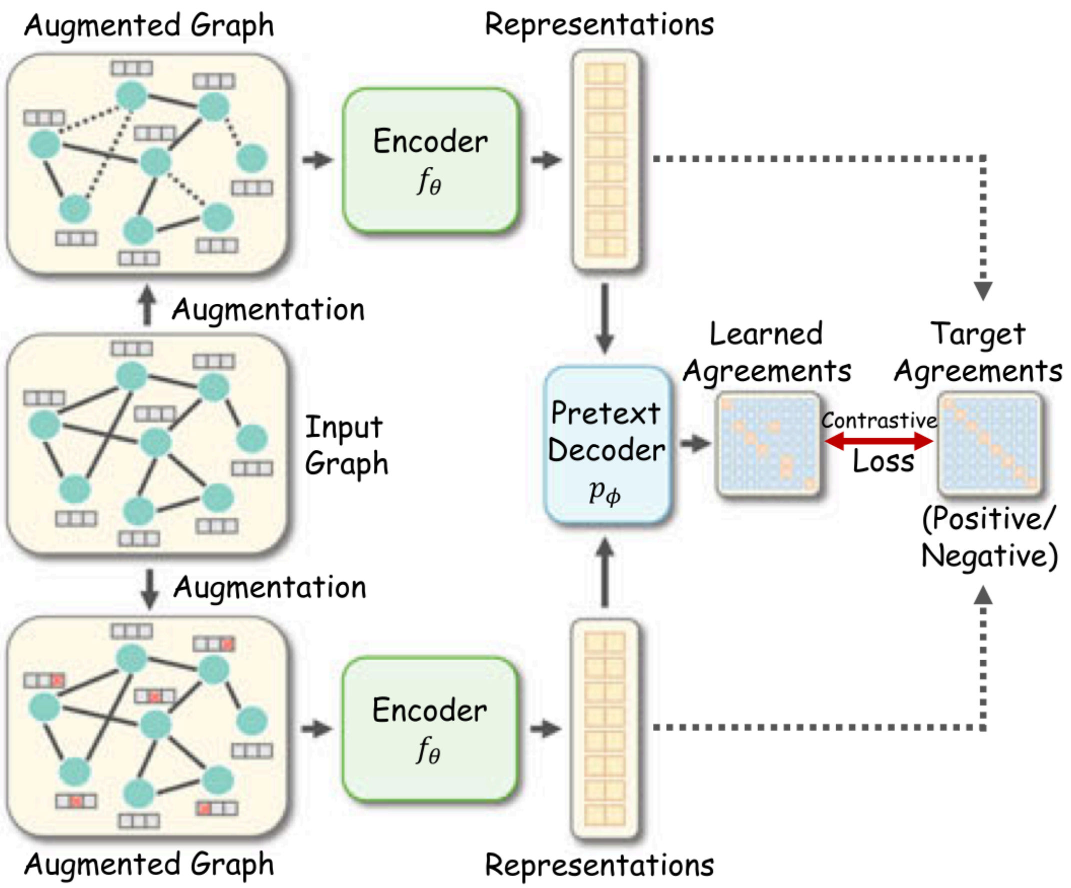
Auxiliary property-based SSL

- Pretext tasks are defined as auxiliary properties of the data (e.g., graph partition, node degree, cluster index)
- It often requires domain knowledge
- The loss is defined to measure the difference between the estimated and the original auxiliary property (e.g., mean square error, cross-entropy)



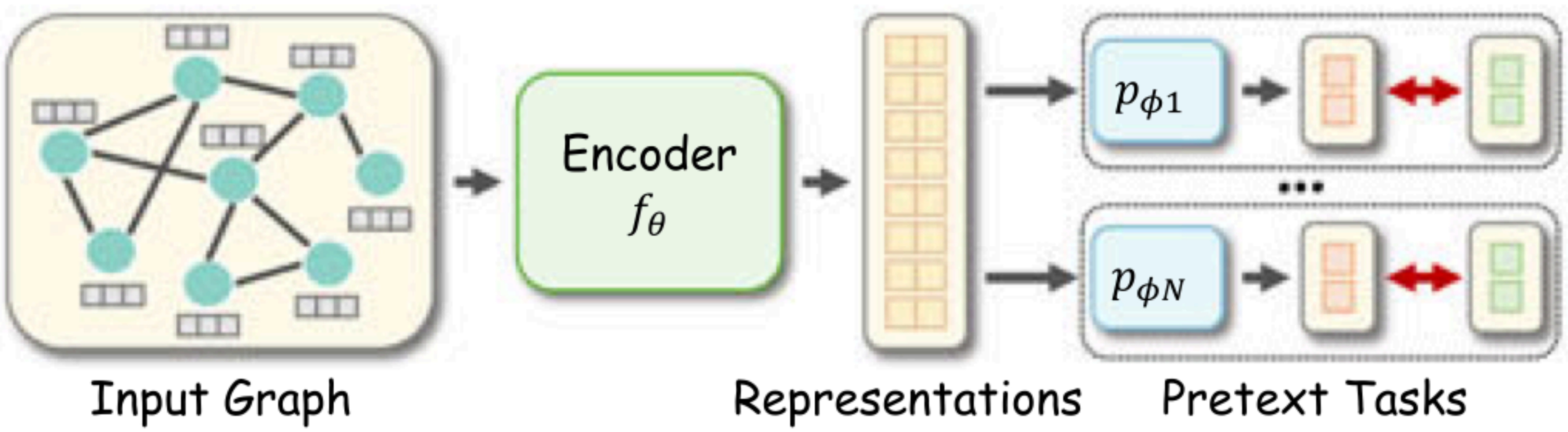
Contrastive-based SSL

- Pretext tasks are defined based on the concepts of mutual information (MI) maximization
- The loss is defined by maximizing the estimated MI between augmented instances of the same object (e.g., node, subgraph, graph)



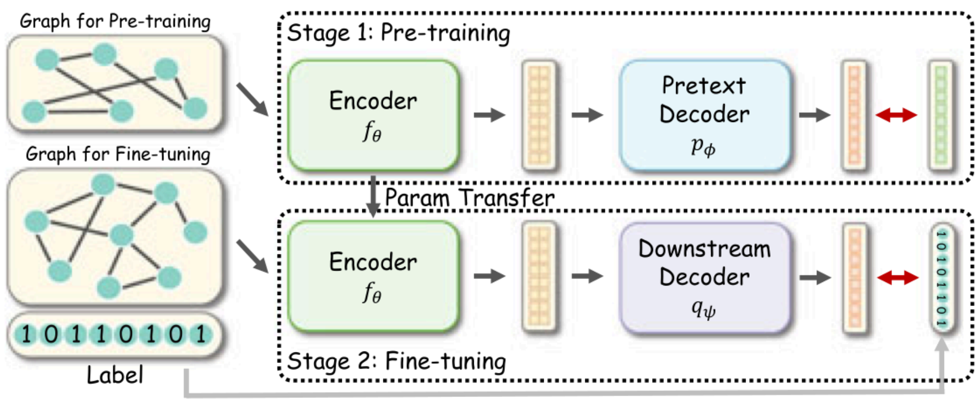
Hybrid methods for SSL

- Pretext tasks are defined based on a combination of multiple objective
- Balancing the different pretext tasks is often challenging

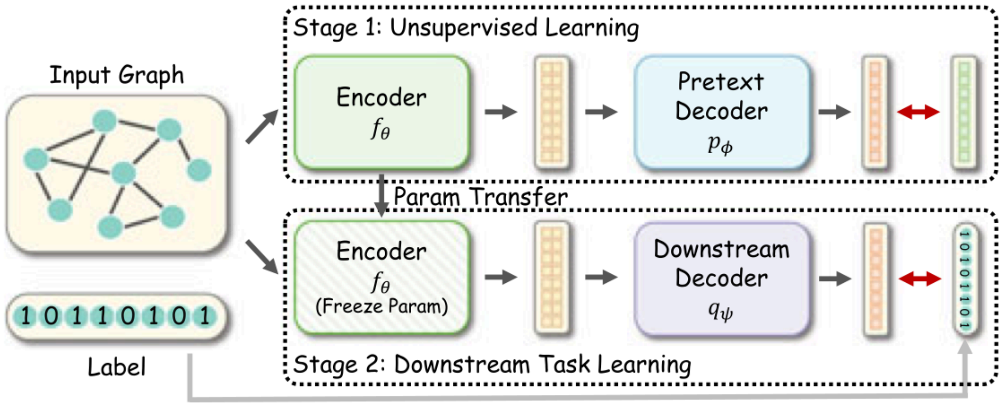


How do I use my labels in SSL?

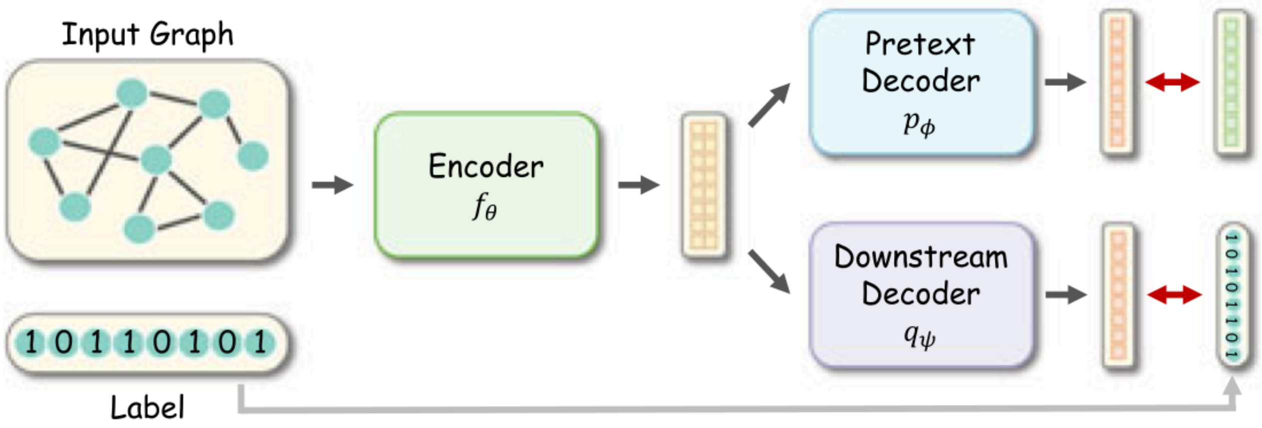
- If labelled data are available, they can be combined with the pretext task(s) to improve the models:



Stage 1: Pre-training on pretext
Stage 2: Fine-tuning on labeled data



Stage 1: Pre-training on pretext
Stage 2: Fine-tuning on labeled data with frozen decoder



Multitask learning: Learn jointly pretext and downstream task

Summary

- The expressive power of GNN architectures has strong connections with the WL kernel
- Building more expressive architectures is still a challenge
- Self-supervised learning on graphs is a promising learning paradigm when labels are limited
- The choice of the pretext task is crucial; It needs to be correlated with the main task

Recall: Useful resources

- **Toolboxes**
  - https://github.com/rusty1s/pytorch_geometric
  - https://github.com/dmlc/dgl
  - https://github.com/deepmind/jraph
  - https://github.com/tensorflow/gnn

- **Datasets**
  - DGL datasets: https://docs.dgl.ai/api/python/dgl.data.html
  - PyG datasets: https://pytorch-geometric.readthedocs.io/en/latest/modules/datasets.html
  - OGB datasets: https://ogb.stanford.edu
  - https://chrsmrrs.github.io/datasets/
  - https://chrsmrrs.github.io/datasets/

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